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Poisson Solver with Floating Conductor Implementation in REMCOM XFDTD Software, Benchmark Calculation Examples

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Poisson Solver with Floating Conductor Implementation in REMCOM XFDTD Software

Benchmark Calculation Examples

Brian R. Poole

Lisa Wang

Introduction:

The XFDTD¹ code produced by REMCOMTM Corp. is a finite difference time domain code used for solution of electromagnetic problems. It has several unique features, including dispersive dielectrics, nonlinear dielectrics and magnetic materials, materials with time dependent conductivity, as well as lumped circuit elements such as inductors, capacitors and resistors. All these features make the code extremely versatile and particularly suited for fully electromagnetic pulse power simulations. One of the characteristics of pulse power simulations is the long charging time of a circuit and the fast discharge of the circuit. In many cases, only the fast discharge needs to be examined from a fully electromagnetic point of view; the charge cycle is usually slow and suitably modeled by conventional circuit techniques. In fact, in many simulations, the time scale of the charge and discharge cycle may vary by over three orders of magnitude. This poses a problem for efficient modeling of the problem, since in reality it is desirable not to model the charge cycle, but only the discharge cycle with the initial conditions defining the initial state of the simulation as established by the charge cycle. This was the motivation to have a Poisson solver introduced into REMCOM's XFDTD code. Using this feature the initial electric field distribution in the simulation geometry could be determined by assigning initial potentials to various conductive structures to set up the initial charge state. This of course meant that there was no initial current flow in the problem, indicating an infinitely long charge cycle. This methodology worked extremely well for many of simulation problems. However, in the first version of this Poisson solver, conductors with unassigned potentials were not allowed; i.e. floating conductors were not allowed. In the latest implementation of the Poisson solver floating conductors with unassigned potentials were introduced into the XFDTD code. In this report, an investigation of the accuracy of the solver is made for a number of representative example geometries in the XFDTD code. To check the validity of the solutions in the test cases, comparisons are made with finite element solutions using the electrostatics solvers using both the COMSOL² TM multi-physics code and the ANSYS/ANSOFT MAXWELL³ TM code. The test cases are designed to exercise the solver in a variety of situations;

- 1) Effect of stair-stepping error introduced by the orthogonal mesh used by XFDTD compared with the finite element mesh used by COMSOL and MAXWELL codes.
- 2) Performance of Poisson solver depending on PEC or open boundary conditions.
- 3) Performance of Poisson solver depending on number of conductors with assigned voltages and number of floating conductors.

- 4) Performance of Poisson solver depending on thin or thick planar structures.
- 5) Accuracy of the Poisson solver depending on whether floating conductors are shielded from the outer boundary condition by other conductors.

It should be noted that the ANSYS/MAXWELL 3D solver does not work with open boundary conditions requiring the user to artificially put the outer boundaries sufficiently far from the region of interest and set the boundary condition to a zero potential boundary condition. Since this method is not well defined, any example that is calculated in unbounded space will exclude the ANSYS/MAXWELL 3D solution in the comparison. Also, the MAXWELL 3D solution was not used in all cases. Also, the source of errors will be discussed in most cases in qualitative general terms, since the purpose of this document is only to provide a guide for the improvement of the Poisson solve in the XFDTD code.

Case 1a)

For the first test case we consider a simple 2 mm radius sphere at +1 Volt potential centered within a 20 mm spherical shell at zero potential as shown in Fig. 1.

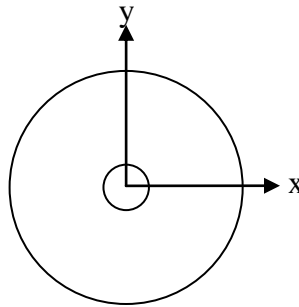


Fig. 1: Simple 2 concentric spheres. Inner sphere radius is 2 mm at +1 V potential, outer sphere radius is 20 mm and at 0 V.

A lineout of the potential along the x axis is plotted in Fig. 2a using the results of XFDTD, COMSOL MultiPhysics, ANSYS Maxwell 3D, as well as an analytic solution for this case. As can be seen in Fig. 2a there is excellent agreement with all three codes and the analytic result with typical errors of -.05%, +0.2%, and +1.9% between the MAXWELL, COMSOL, and XFDTD with the analytic results respectively. The larger error associated with the XFDTD code is primarily due to stair-stepping error in this case.

Case 1b)

For this case we consider a 2 mm sphere at +1 V potential in unbounded space. Figure 2b shows the comparison of results for this case with the analytic result. Several different cell sizes were used for the XFDTD solution. As can be seen, the COMSOL result agrees extremely well with the analytic result with a typical error of less than 0.02%, while the XFDTD results agree reasonably well near the sphere but deviate significantly near the outer regions. Errors evaluated at a distance of $x = 15$ mm show relative errors of 70%, 15%, and 40% for XFDTD cubical cell

sizes of 0.1 mm, 0.2 mm, and 0.075 mm respectively. Based on the fact that the accuracy is reasonable near the sphere and the fact that the results were globally accurate for the sphere enclosed in a grounded spherical shell (Case 1a) would indicate that stair-stepping inaccuracies are not that significant in this case, and the performance of the open boundary in the XFDTD Poisson solver is problematic. Also, it seems that the accuracy has an oscillatory convergence.

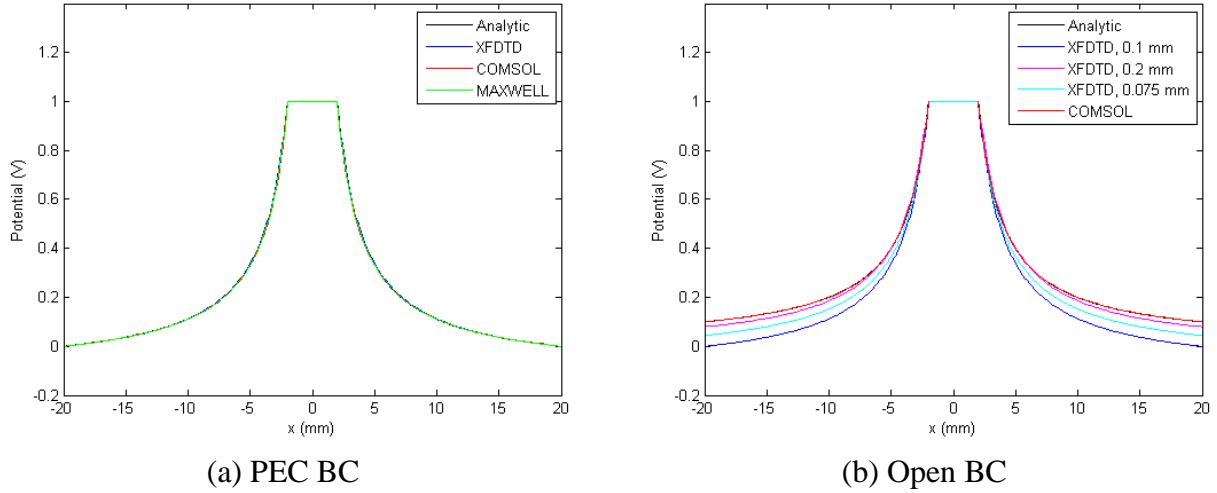


Fig. 2: Comparison of XFDTD, COMSOL, MAXWELL, and analytic results for test Case 1a and XFDTD, COMSOL, and analytic results for Case 1b.

Case 2a)

In this case we consider two 2 mm radius spheres within a 20 mm spherical shell at zero potential as shown in Fig. 3. The y and z centers of the conducting spheres are both at zero. The x location of the first sphere is at $x = -4$ mm and at a potential of -1 V and the second sphere as at +4 mm with a potential of +1 V. The outer spherical shell is centered at the origin.

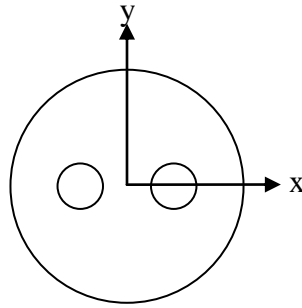


Fig. 3: Two 2 mm radius spheres located within 20 mm outer sphere. The two interior spheres are centered at -4 mm and +4 mm. The left sphere is at a potential of -1 V and the right sphere is at a potential of +1 V. The outer sphere is at zero potential.

A lineout of the potential along the x axis is plotted in Figs. 4a using the results of XFDTD, COMSOL MultiPhysics, and ANSYS Maxwell 3D. Figure 4a also shows vertical lineouts in y of

the potential through the centers of the 2 small interior spheres at $x = -4$ mm and $x = +4$ mm respectively. As can be seen in Figs. 4a there is excellent agreement between all three codes; COMSOL and MAXWELL 3D give nearly identical results with typical differences being on the order of 2% between COMSOL or MAXWELL 3D and XFDTD.

Case 2b)

Case 2b is identical to Case 2a except that the 20 mm conducting shell was removed and the two small spheres were located in unbounded space. Figures 4b shows the results for the same three lineouts as in Case 2a. Again, there is excellent agreement between COMSOL and XFDTD, with typical a typical difference of 2%. The difference provides some insight into the performance of the open boundary condition used in Case 1b and Case 2b. Case 1b generated fairly inaccurate results compared with Case 2b; the primary difference being that Case 2b had balanced potentials on the two spheres while Case 1b has an unbalanced potential.

Case 3a)

Case 3a is identical to Case 2a, except that the interior sphere at $x = 4$ mm is at a potential of +2 V. The outer shell is at zero potential. Figures 5a shows the results for the same three lineouts as in Case 2a.

Case 3b)

Case 3b is identical to Case 3a, except there is no exterior conducting shell in this case. Figures 5b show the results for the same three lineouts as in Case 2a.

Case 4a)

Case 4a is identical to Case 2a, except that the interior sphere at $x = -4$ mm is at an unassigned potential, i.e., the sphere is floated. The interior sphere at $x = 4$ mm is at a potential of +1 V. The outer shell is at zero potential. Figures 6a show the results for the same three lineouts as in Case 2a.

Case 4b)

Case 4b is identical to Case 4a, except there is no exterior conducting shell in this case. Figures 6b show the results for the same three lineouts as in Case 2a.

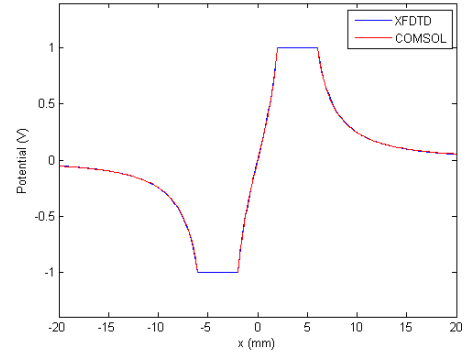
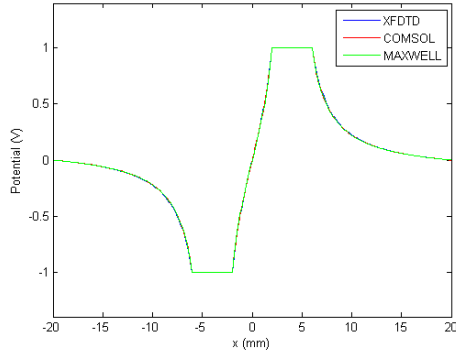
Case 5a)

Case 5a is identical to Case 2a, except that the interior sphere at $x = +4$ mm has a radius of 4 mm. The outer shell is at zero potential. Figures 7a show the results for the same three lineouts as in Case 2a.

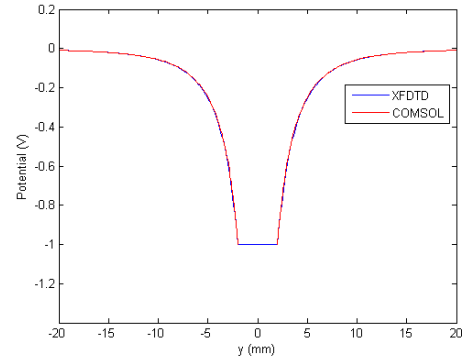
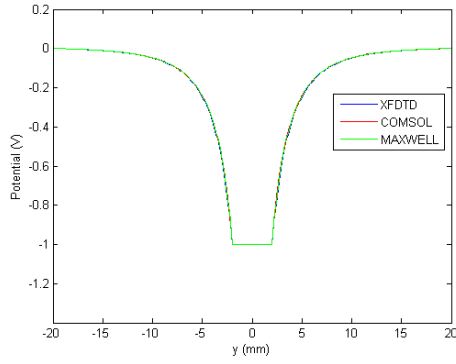
Case 5b)

Case 5b is identical to Case 5a, except there is no exterior conducting shell in this case. Figures 7b show the results for the same three lineouts as in Case 2a.

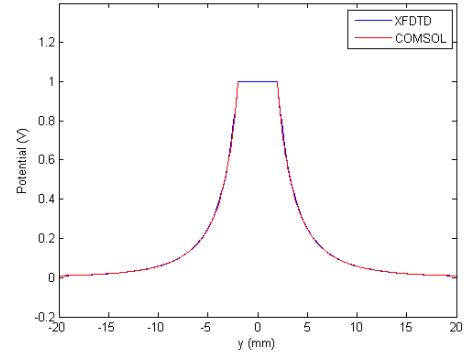
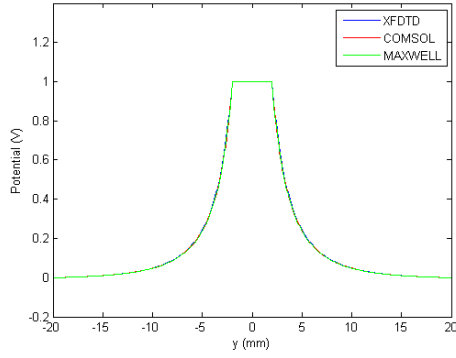
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lineout
y = 0



y
lineout
x = -4
mm



y
lineout
x = +4
mm

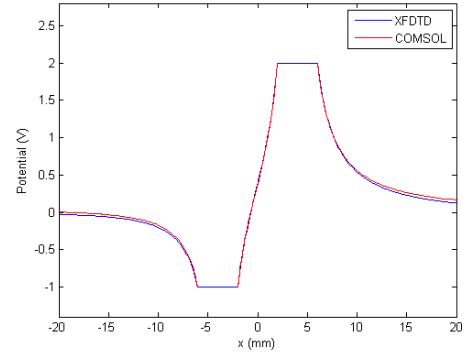
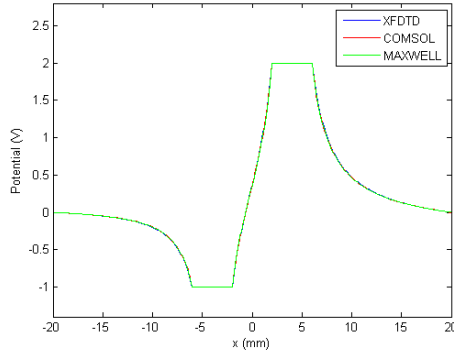


(a) PEC BC

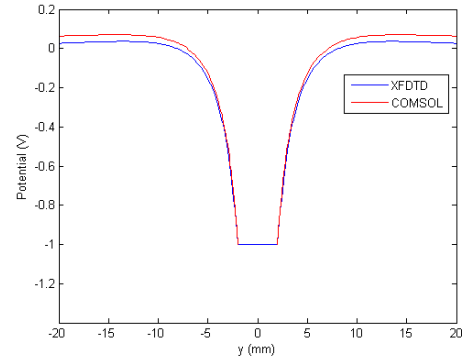
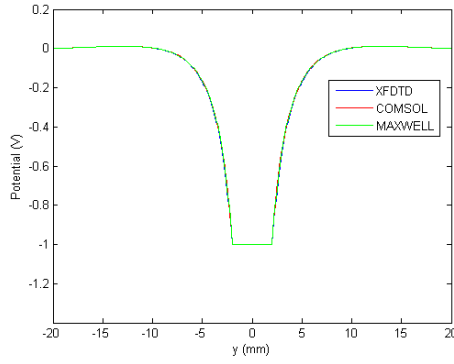
(b) Open BC

Fig. 4: Comparison of XFDTD, COMSOL, MAXWELL, and analytic results for test Case 2a and XFDTD, COMSOL, and analytic results for Case 2b.

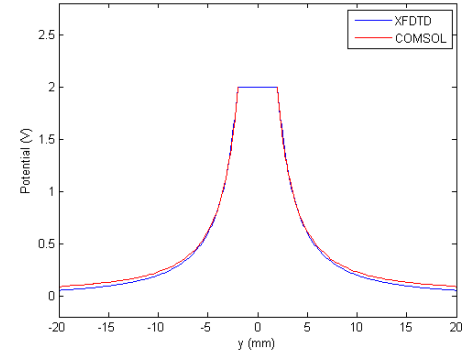
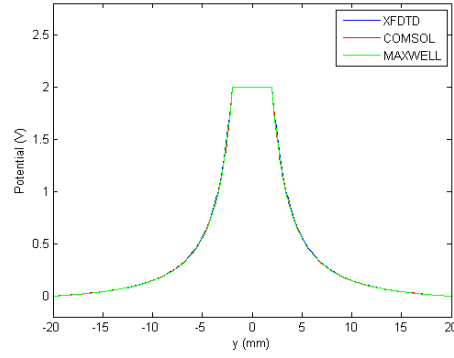
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y
lineout
x = -4
mm



y
lineout
x = +4
mm

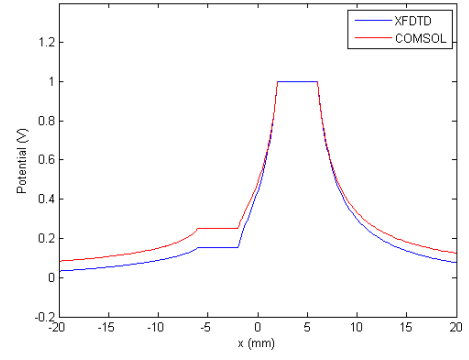
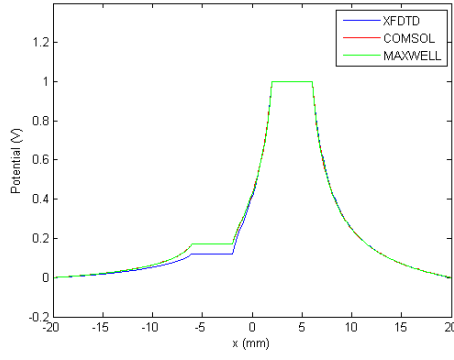


(a) PEC BC

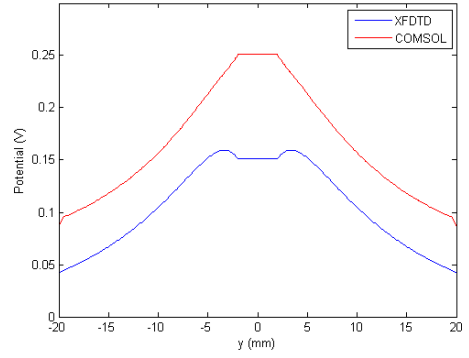
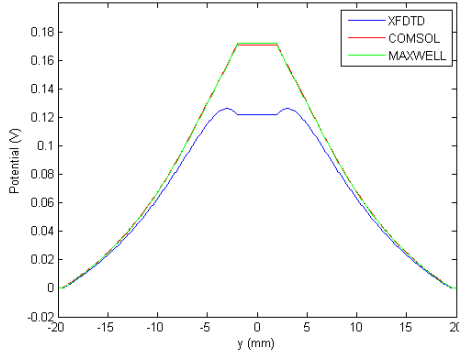
(b) Open BC

Fig. 5: Comparison of XFDTD, COMSOL, MAXWELL, and analytic results for test Case 3a and XFDTD, COMSOL, and analytic results for Case 3b.

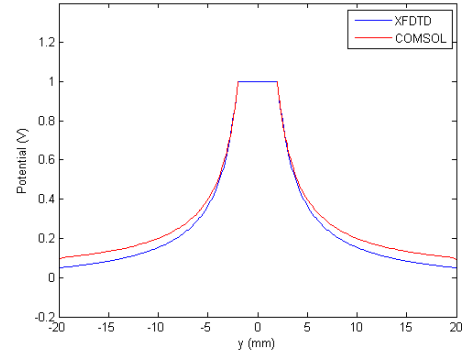
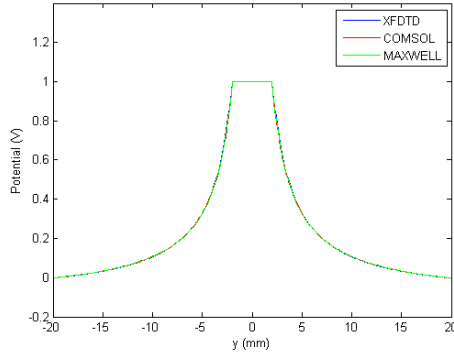
x
lineout
y = 0



y
lineout
x = -4
mm



y
lineout
x = +4
mm



(a) PEC BC

(b) Open BC

Fig. 6: Comparison of XFDTD, COMSOL, MAXWELL, and analytic results for test Case 4a and XFDTD, COMSOL, and analytic results for Case 4b.

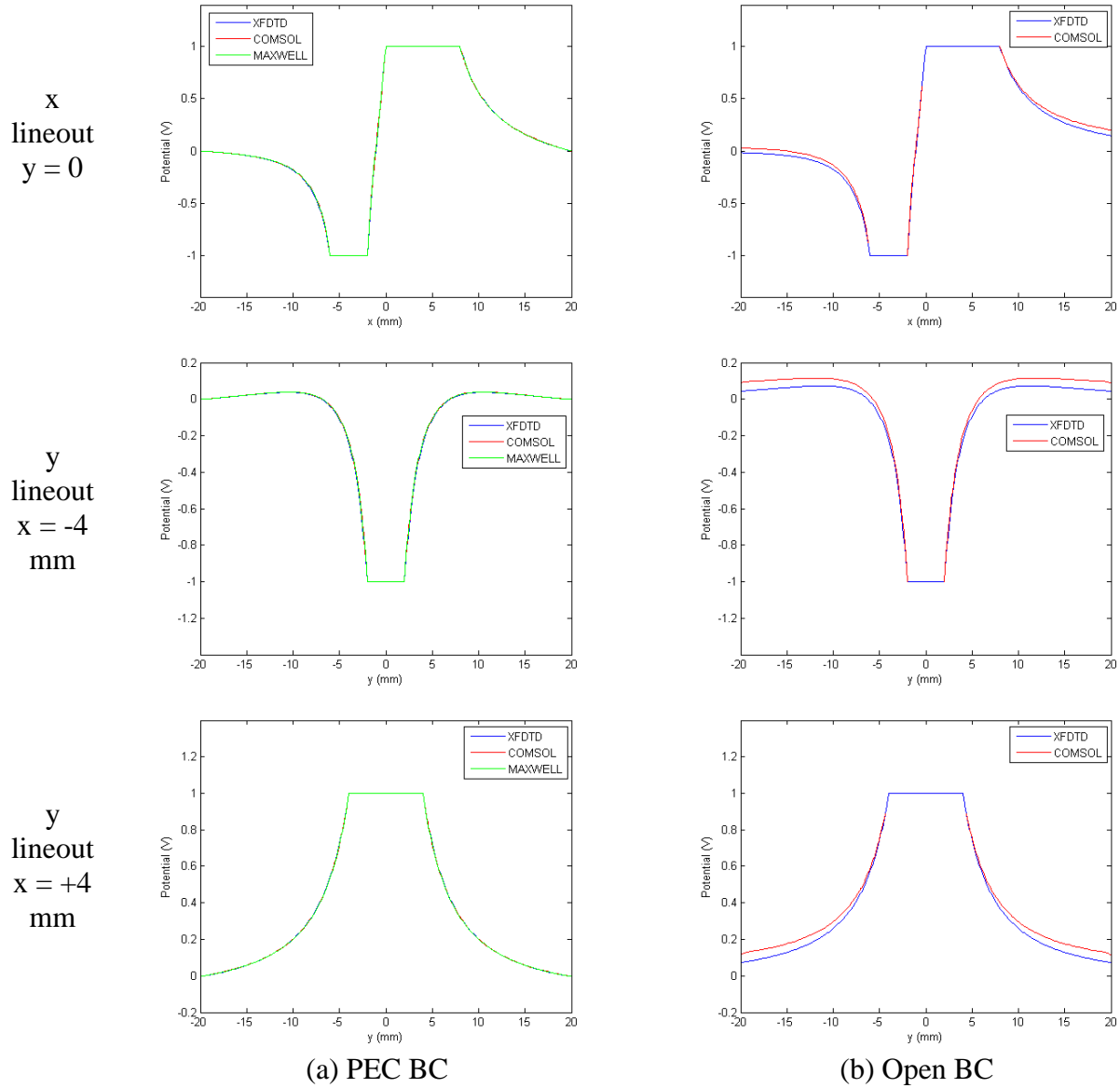


Fig. 7: Comparison of XFDTD, COMSOL, MAXWELL, and analytic results for test Case 5a and XFDTD, COMSOL, and analytic results for Case 5b.

Cases 3 through 5 demonstrated that the XFDTD Poisson solver performed very well with an outer PEC boundary and no floating conductors. When a floating conductor was introduced localized relative errors on the order of 30% were introduced at or near the floating conductor. The solution was still reasonably accurate near conductors with assigned potentials. When an open boundary condition was introduced, relative errors on the order of 50% still persisted near the outer boundary but the overall error was dramatically increased at and near the floating conductor. The size of the interior spheres does not seem to significantly change the relative error.

Case 6a)

In this case we consider three spheres within a rectangular box as shown in Fig. 8. The dimensions of the box are from $x = -8$ mm to 8 mm, $y = -5$ mm to 5 mm, and $z = -4$ mm to 4 mm. Sphere, S1 has a radius of 1 mm, centered at $(x,y,z) = (-5,1,0)$ mm, sphere, S2 has a radius of 1 mm, centered at $(x,y,z) = (-2,-3,0)$ mm, and sphere, S3 has a radius of 2 mm, centered at $(x,y,z) = (4,-0.5,0)$ mm. Sphere 1 is at a potential of -1 V, sphere 2 is at a floating potential, and sphere 3 is at a potential of $+2$ V. The outer rectangular box is at zero potential. Lineouts in x and y , through the centers of each of the spheres are shown in Figs. 9a and 10a.

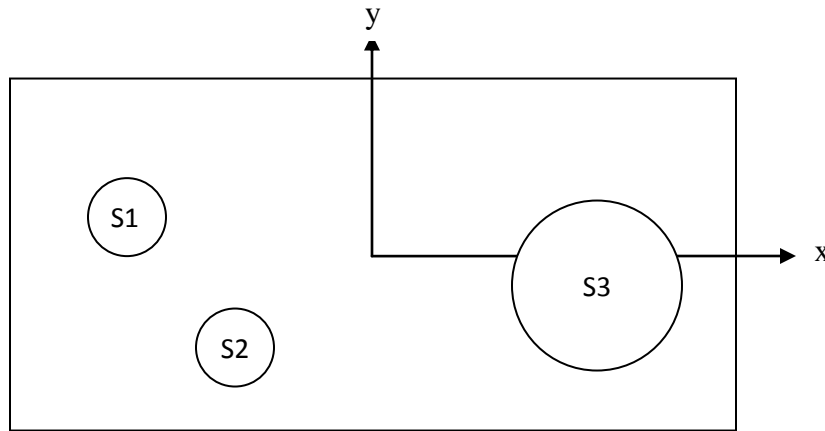


Fig. 8: Three spheres located within rectangular box as described in Case 6a. Lineouts in x and y are determined through the x and y centers of each of the three spheres.

Case 6b)

Case 6b is identical to Case 6a except that the conducting rectangular box was removed and the three spheres were located in unbounded space. Figures 9b and 10b show the results for the same three lineouts as in Case 6a.

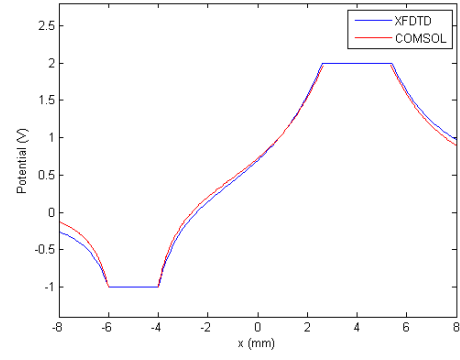
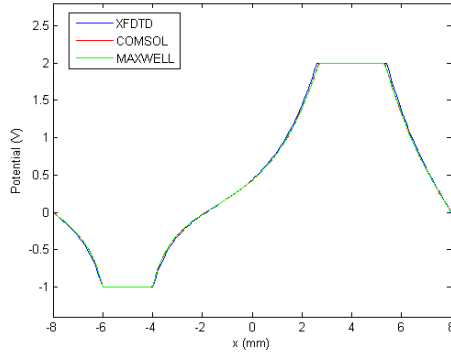
Case 7a)

Case 7a is identical to Case 6a except that the three spheres were replaced with cubes centered at the same locations as the spheres with their edge lengths being the same as the sphere diameters. Maxwell results not available for this case. Figures 11a and 12a show the results for the same three lineouts as in Case 6a.

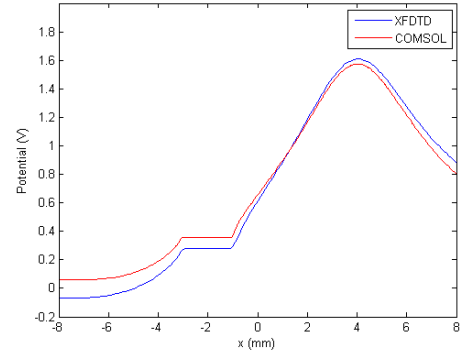
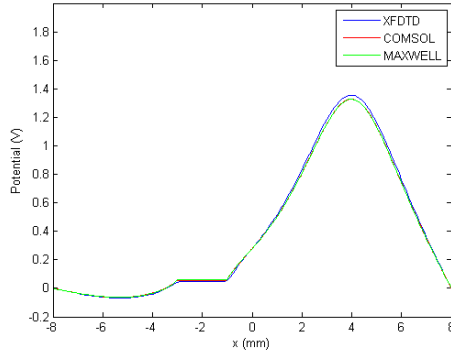
Case 7b)

Case 7b is identical to Case 7a except that the conducting rectangular box was removed and the three cubes were located in unbounded space. . Figures 11b and 12b show the results for the same three lineouts as in Case 6a.

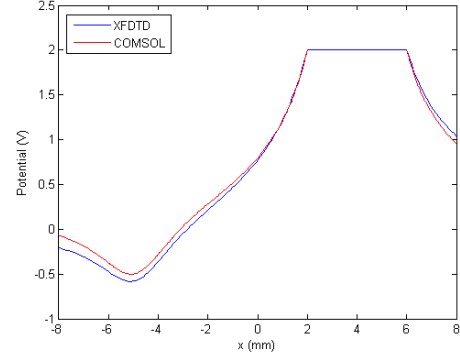
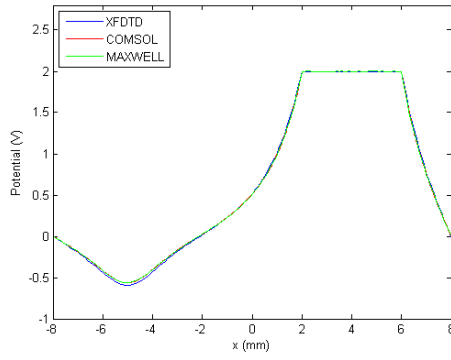
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lineout
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x
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y = -3
mm



x
lineout
y = -.5
mm

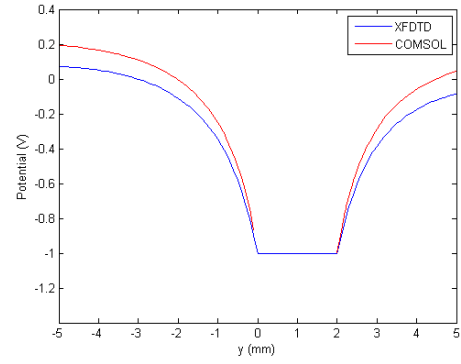
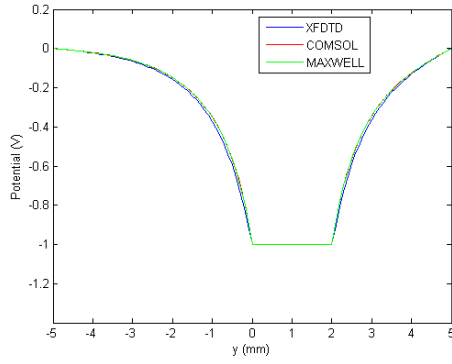


(a) PEC BC

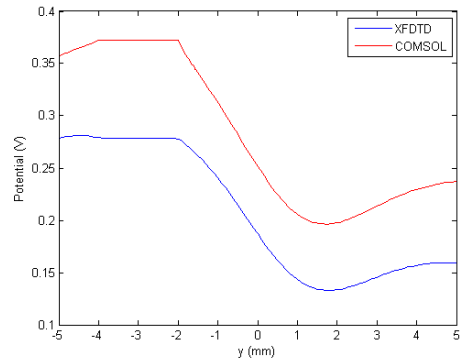
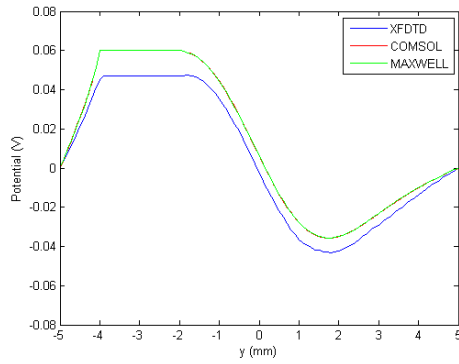
(b) Open BC

Fig. 9: Comparison of XFDTD, COMSOL, MAXWELL, and analytic results for test Case 6a and XFDTD, COMSOL, and analytic results for Case 6b.

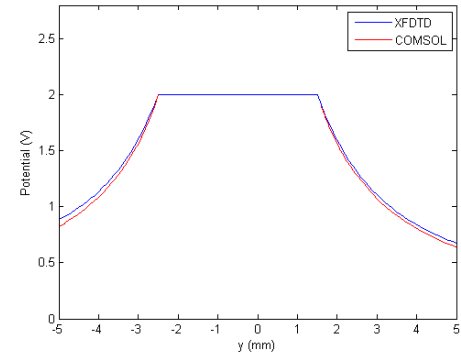
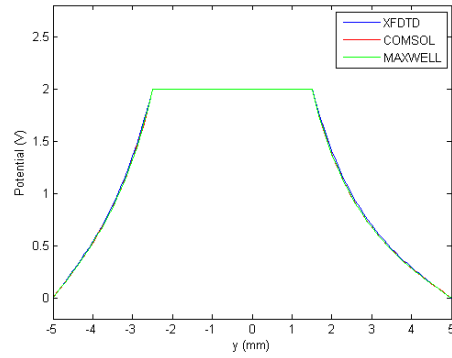
y
lineout
x = -5
mm



y
lineout
x = -2
mm



y
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x = +4
mm

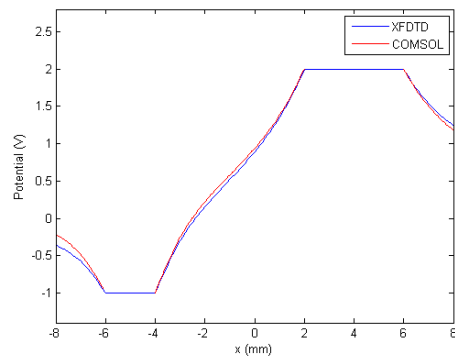
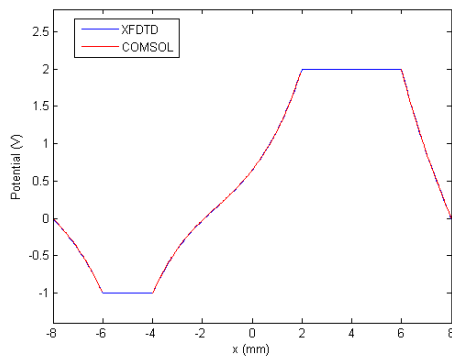


(a) PEC BC

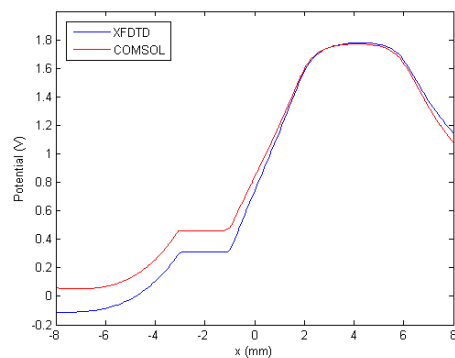
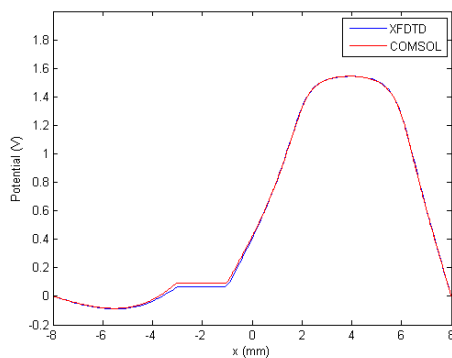
(b) Open BC

Fig. 10: Comparison of XFDTD, COMSOL, MAXWELL, and analytic results for test Case 6a and XFDTD, COMSOL, and analytic results for Case 6b.

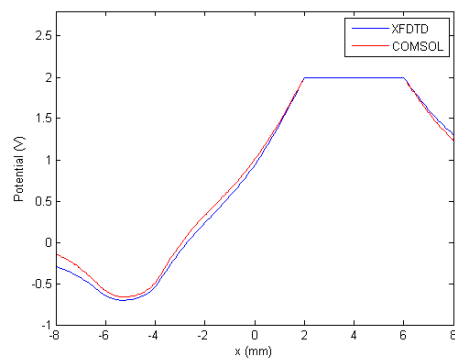
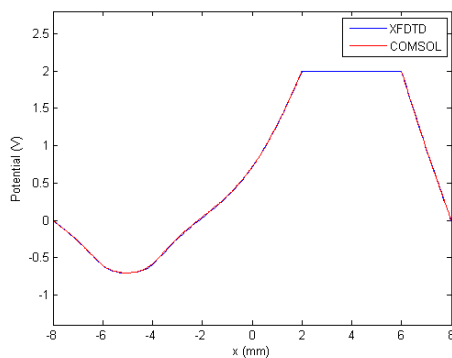
x
lineout
y = 1
mm



x
lineout
y = -3
mm



x
lineout
y = -.5
mm



(a) PEC BC

(b) Open BC

Fig. 11: Comparison of XFDTD and COMSOL, for test Case 7a and Case 7b.

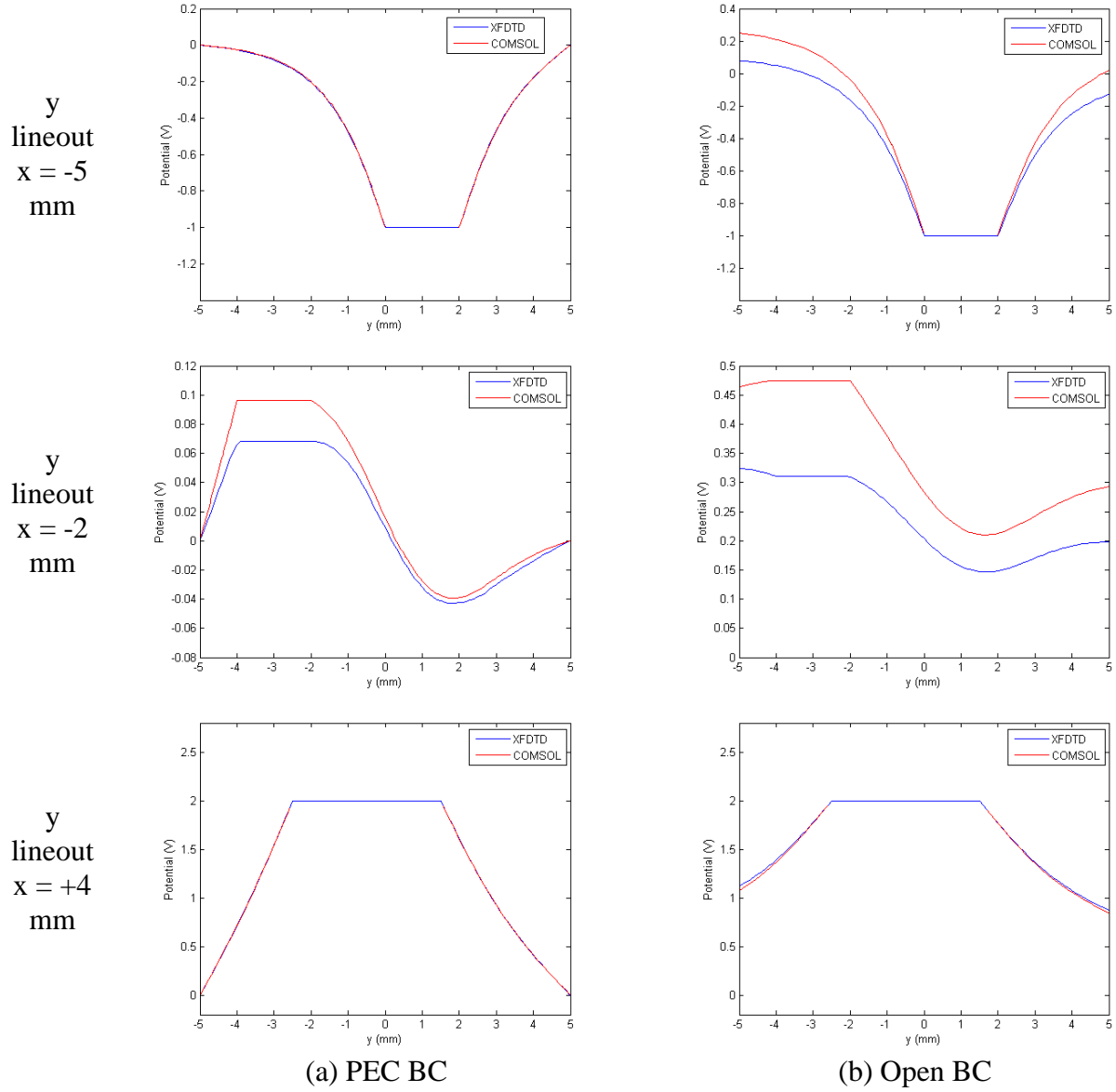


Fig. 12: Comparison of XFDTD and COMSOL, for test Case 7a and Case 7b.

Cases 6 and 7 again demonstrate that the XFDTD Poisson solver performed very well with an outer PEC boundary and no floating conductors. The introduction of a floating conductor again introduced large relative errors in the vicinity of the floating conductor and subsequently with the introduction of an open boundary condition made the errors significantly worse. As before, the solution retained accuracy near the objects with a specified potential. The worst case situation would be placing a floating conductor too close to an open boundary condition. Errors were comparable between the three sphere cases and the three cube cases indicating that stair-stepping error was not the source of the inaccuracies since stair-stepping was not present in the mesh associated with the three cube problem. Almost certainly, the open boundary condition and the method used to determine the potential of the floating object were the primary source of error.

Case 8a)

In this case we consider three infinitely thin square perfectly conducting plates with an edge length of 40 mm. The three plates are located at $y = -1$, -0.5 and $+1$ mm. The plate at -1 mm and $+1$ mm are at potential of -1 V and $+1$ V respectively. The plate at $y = -0.5$ mm is floated. The three plates are in a perfectly conducting rectangular box at zero potential with dimensions of 60 mm in x , 60 mm in z , and 6.6 mm in y with the center of the box at the origin as shown in Fig. 13. Lineouts of the potentials along the x axis midway between the plates at $y = -0.75$ mm, $y = 0.25$ mm, and the y axis at $x = 0$. The lineouts are always in the $z = 0$ plane. Figure 14a show the results of these lineouts.

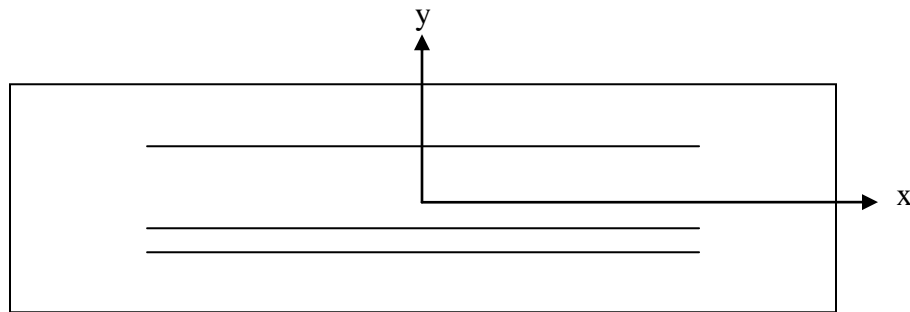
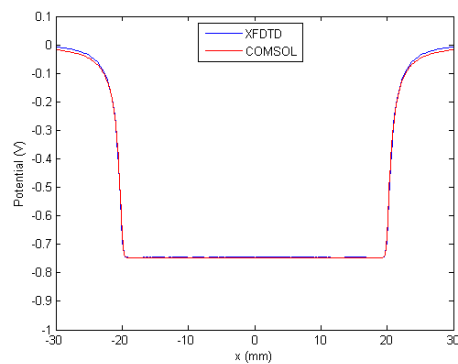
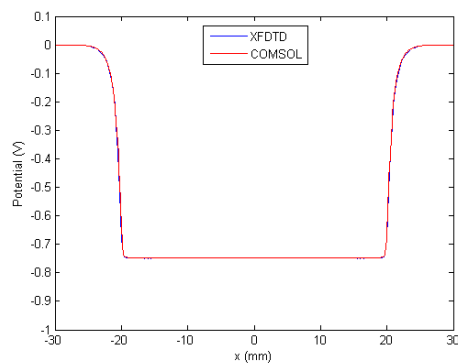


Fig. 13: Three plate capacitor problem described in Case 8a.

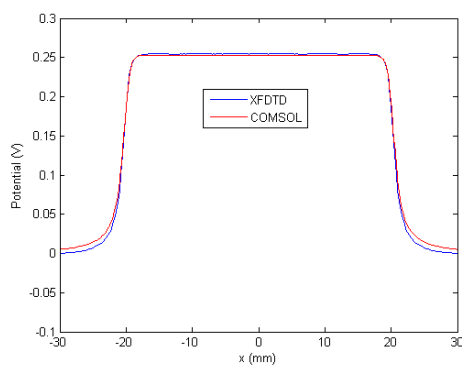
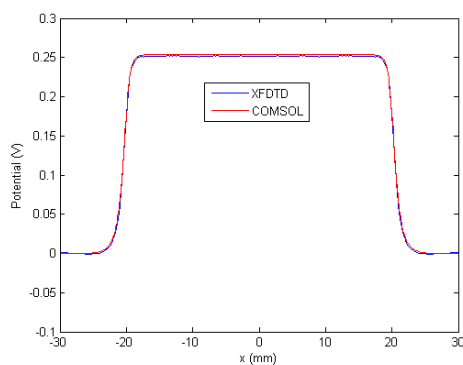
Case 8b)

Case 8b is identical to Case 8a except that the conducting rectangular box was removed and the three plates were located in unbounded space. Figures 14b show the results for the same three lineouts as in Case 8a.

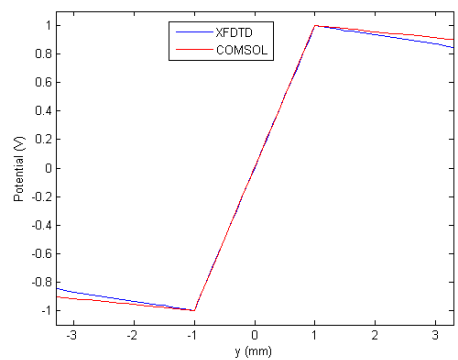
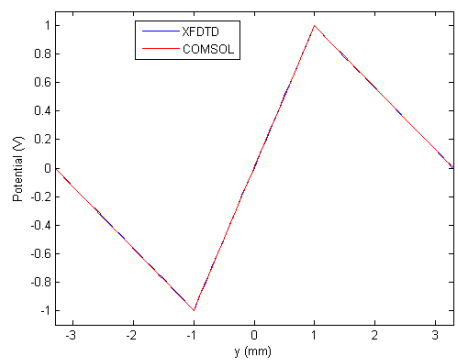
x
lineout
y = -.75
mm



x
lineout
y = .25
mm



y
lineout
x = 0
mm



(a) PEC BC

(b) Open BC

Fig. 14: Comparison of XFDTD and COMSOL, for Case 8a and Case 8b.

Case 9a) and 9b)

In this case we consider a capacitor using multiple interleaved segmented plates in a serpentine configuration designed to minimize inductance as shown in Fig. 15. All the plates are of zero thickness. This type of capacitor structure is designed to minimize inductance. The external connections were set to potentials of -1 V and $+1\text{ V}$. This model was included to examine the performance with multiple floating plates. The region indicated in blue is a dielectric with a relative dielectric constant of 2000. For Case 9a the capacitor is enclosed in a PEC rectangular box and for Case 9b the outer box is removed for a calculation with open boundary conditions.

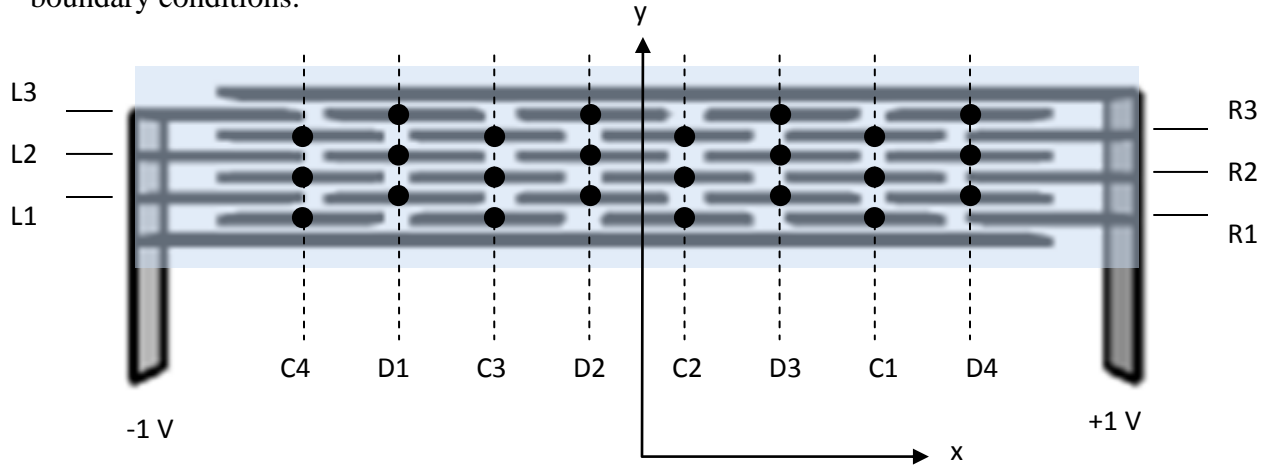


Fig 15: Segmented capacitor shown with sample points for evaluating floating potentials.

The dimensions of the dielectric block are 50 mm in x, 50 mm in z, and 10 mm in y. The origin of the coordinate system is in the center of the block. The dimensions of the outer PEC boundary for Case 9a are 100 mm in x, 100 mm in z and 40 mm in y. Each of the floating electrodes has dimensions of 47 mm in y and 7 mm in x, with 2 mm spacing between electrodes on the same layer. Layer to layer spacing is 1 mm. Figure 15 shows the potential distribution in the capacitor.

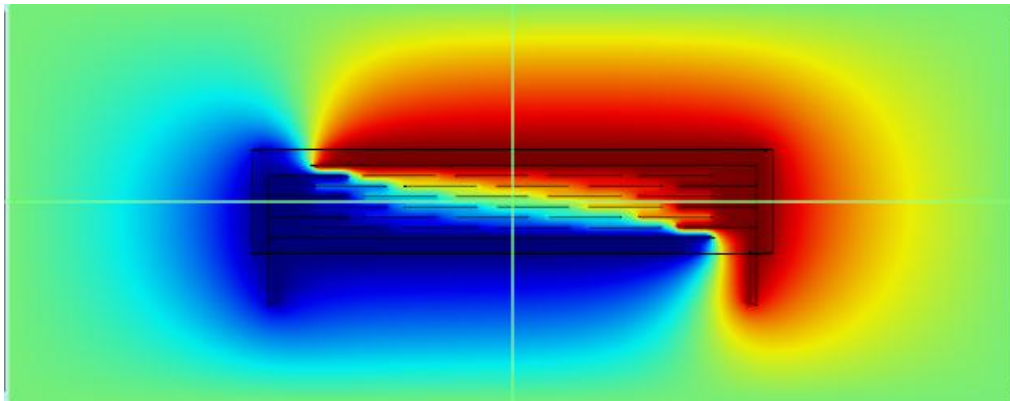


Figure 16: Potential distribution in the capacitor.

Table 1 shows the values of the floating potentials for Case 9a for COMSOL and XFDTD simulations, and Table 2 shows the floating potentials for Case 9b for the COMSOL and XFDTD simulations.

Location	COMSOL	XFDTD	Relative Error
Coordinate	Potential (V)	Potential (V)	Percent %
R1 – C1	-0.4634	-0.4524	-2.37
R1 – C2	-0.6779	-0.6717	-0.91
R1 – C3	-0.7937	-0.7898	-0.49
R1 – C4	-0.9318	-0.9280	-0.41
L1 – D1	-0.6899	-0.6885	-0.20
L1 – D2	-0.4619	-0.4582	-0.80
L1 – D3	-0.2166	-0.2073	-4.29
L1 – D4	+0.4850	+0.4930	+1.65
R2 – C1	+0.2944	+0.3025	+2.75
R2 – C2	-0.0810	-0.0780	-3.70
R2 – C3	-0.3576	-0.3600	+0.67
R2 – C4	-0.7754	-0.7747	-0.09
L2 – D1	-0.2945	-0.3052	+3.63
L2 – D2	+0.0810	+0.0753	-7.04
L2 – D3	+0.3575	+0.3573	-0.06
L2 – D4	+0.7755	+0.7732	-0.30
R3 – C1	+0.6899	+0.6866	-0.48
R3 – C2	+0.4619	+0.4561	-1.26
R3 – C3	+0.2166	+0.2050	-5.36
R3 – C4	-0.4847	-0.4947	+2.06
L3 – D1	+0.4634	+0.4511	-2.65
L3 – D2	+0.6779	+0.6705	-1.09
L3 – D3	+0.7937	+0.7886	-0.64
L3 – D4	+0.9318	+0.9273	-0.48

Table 1: Floating potentials for Case 9a.

Location	COMSOL	XFDTD	Relative Error
Coordinate	Potential (V)	Potential (V)	Percent %
R1 – C1	-0.4635	-0.4524	-2.39
R1 – C2	-0.6779	-0.6718	-0.90
R1 – C3	-0.7937	-0.7901	-0.45
R1 – C4	-0.9318	-0.9283	-0.38
L1 – D1	-0.6899	-0.6888	-0.16
L1 – D2	-0.4619	-0.4585	-0.74
L1 – D3	-0.2166	-0.2073	-4.29
L1 – D4	+0.4849	+0.4932	+1.71
R2 – C1	+0.2945	+0.3028	+2.82
R2 – C2	-0.0809	-0.0779	-3.71
R2 – C3	-0.3576	-0.3602	0.73
R2 – C4	-0.7755	-0.7748	-0.09
L2 – D1	-0.2944	-0.3053	+3.70
L2 – D2	+0.0810	+0.0754	-6.91
L2 – D3	+0.3575	+0.3577	0.06
L2 – D4	+0.7755	+0.7735	-0.26
R3 – C1	+0.6899	+0.6870	-0.42
R3 – C2	+0.4619	+0.4564	-1.19
R3 – C3	+0.2167	+0.2052	-5.31
R3 – C4	-0.4847	-0.4947	+2.06
L3 – D1	+0.4635	+0.4512	-2.65
L3 – D2	+0.6779	+0.6706	-1.08
L3 – D3	+0.7936	+0.7889	-0.59
L3 – D4	+0.9318	+0.9277	-0.44

Table 2: Floating potentials for Case 9b.

Conclusions:

A set of benchmark calculations were performed using the COMSOL, MAXWELL_3D, and XFDTD electromagnetic software tools to aid in evaluating the performance of the XFDTD, static Poisson solver. While not intended to be an exhaustive examination of the codes, the various calculations were used to exercise the XFDTD code for a variety of conditions that may present themselves to the user. The qualitative observations for the XFDTD Poisson solver are summarized below.

- 1) XFDTD produced reasonable accurate results for all geometries that did not have floating conductors or open outer boundary conditions, assuming the mesh had sufficient geometric fidelity to resolve the geometrical features of the model.
- 2) With the introduction of open outer boundary conditions, and no floating conductors, XFDTD produced reasonably accurate results only in regions sufficiently far from the open boundaries. This is a reasonable expectation, since the outer open boundary

condition in XFDTD is designed for time domain electromagnetic problems, not the solution of Laplace's equation in the domain.

- 3) With the introduction of a single floating conductor, significant relative errors occurred in the vicinity of the floating conductor, even with PEC boundary conditions, especially if the induced potential on the floating conductor was close to zero.
- 4) With the introduction of open boundaries and floating conductors inaccuracies were significant in the vicinity of the floating conductor especially if the floating conductor could "see" the open boundary, i.e. was not shielded from the open boundary by conductors with assigned potentials. This result was apparent in the simulation involving the three spheres or cubes (Cases 6 and 7). Since the errors were comparable between the cases with spheres and the equivalent cases with spheres, it is reasonable to assume that the errors were not due to stair-stepping errors and were primarily due to error due to the open boundary and errors in determining the induced potential on the floating conductor.
- 5) The three plate and multi-plate capacitor performed well with the floating conductors and with either PEC or open boundaries since the floating plates were well shielded from the outer boundary, and the floating structures were very close to surrounding structures with assigned potentials. This produced fairly accurate results for both these cases.

References:

- 1) XFDTD is a product of REMCOM Inc., 315 South Allen Street, Suite 416, State College, PA 16801 USA, www.remcom.com
- 2) COMSOL Multiphysics is a product of COMSOL Inc., 1 New England Executive Park, Suite 350, Burlington, MA 01803 USA, www.comsol.com
- 3) MAXWELL is a product of ANSYS Inc., 275 Technology Drive, Canonsburg, PA 15317 USA, www.ansys.com